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Shock-induced alpha-omega structural phase transformation of titanium: A molecular-dynamics study

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Shock-induced α-ω structural phase transformation of titanium: A molecular-dynamics study

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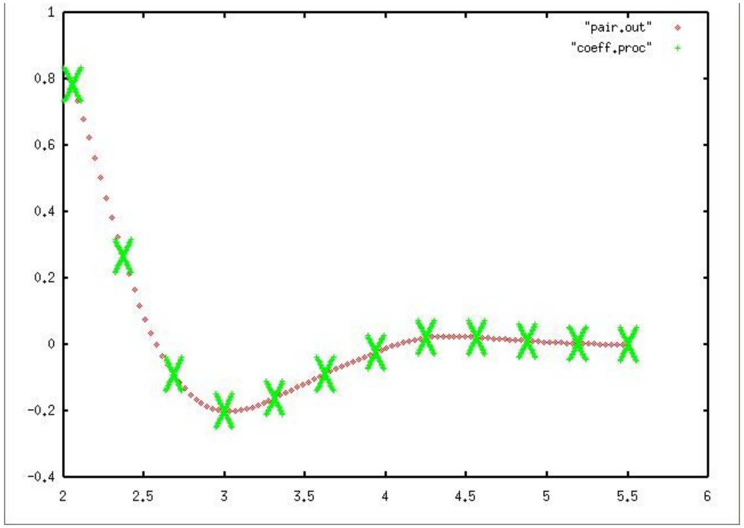
Outline

- Introduction – interatomic potentials, MEAM
- **Ti** – phase transformation
- Molecular-dynamics simulations of the shock-induced phase transformation of Ti.

MEAM Model Form

$$E_{tot} = \sum_{ij} \phi(r_{ij}) + \sum_{i} U(x_i)$$

$$x_i = \sum_{j} \rho(r_{ij}) + \sum_{jk} f(r_{ij}) f(r_{ik}) g(\cos(\theta_{jik}))$$



The various terms are represented by splines with many degrees of freedom, allowing much greater accuracy.

Two and three-body terms are summed over nearby atoms

Fitting Database

- **Energies**
  → for different crystal phases E(V)
  → Vacancy/Interstitial energies
  → Surfaces, clusters, other energies
- **Forces** – force matching method of Ercolessi and Adams
  → snapshots from MD
  → crystal with random displacements
- **Elastic constants and phonons**

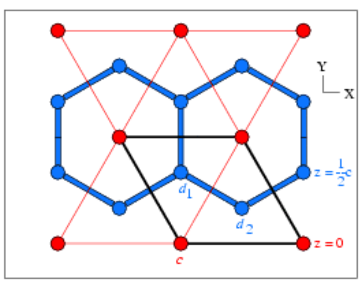
Titanium Phases

We want a model that describes α-ω Transitions

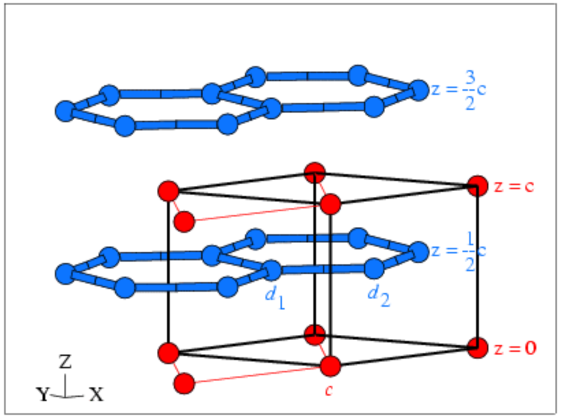
→Pathways for phase transformation
→Kinetics of moving interface, shock physics
→Atomic structure of moving interface

Hexagonal ($P6/mmm$) cell with 3 atoms

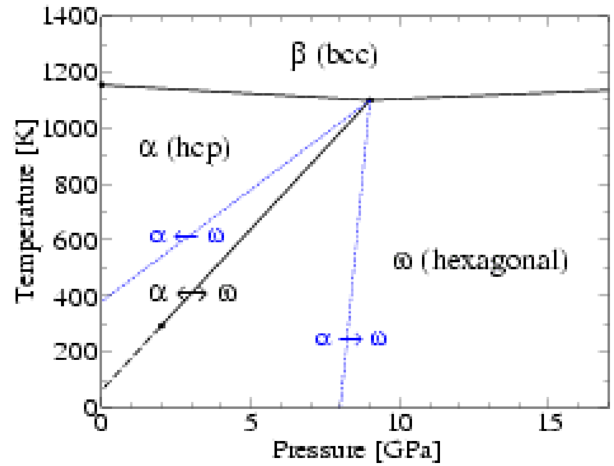
Prototype: MgB_2 structure



omega viewed along c axis



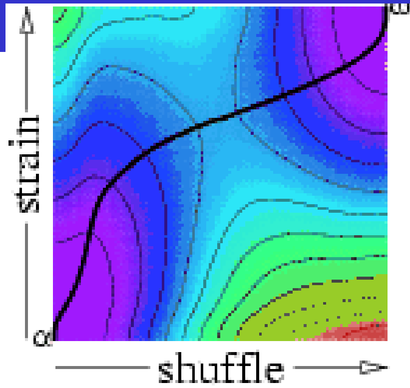
omega with exaggerated c axis (side view)



α is hcp (sphere packing)
but ω is a more complex phase

Ti Phase Transformation Barriers

D. R. Trinkle et al, Phys Rev Lett 91(2) 025701-1 (2003)



In this study pathways were systematically enumerated for Ti.

Each pathway consists of *shuffle* (atomic displacements within cell) and *strain* (changing shape of cell). Both are linearly interpolated.

Landscape barrier: Barrier in 2-D shuffle/strain plot

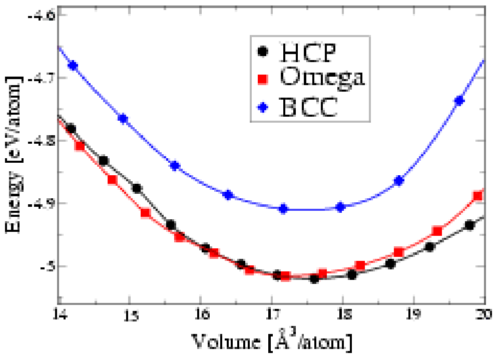
Actual barriers can then be found by relaxing atoms along path.

We want MEAM to predict correct barriers, landscape barriers used as test.

MEAM Potential for Titanium

- Classical model (Modified embedded-atom) of form used by T. Lenosky, et al.
- Parameterized to fit VASP crystal data, surface energies, and defect energies and forces

- **Total Energy**

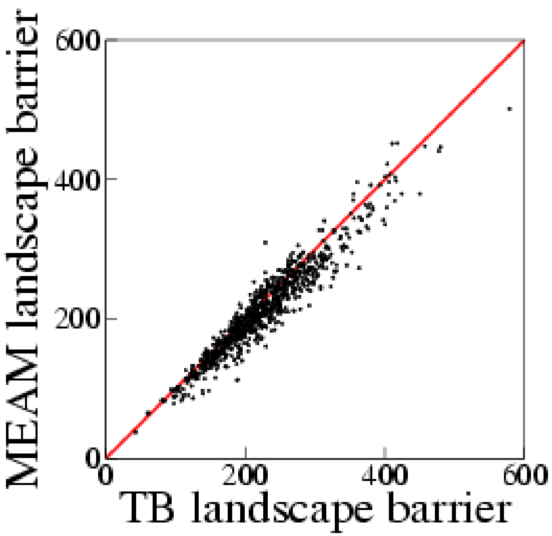


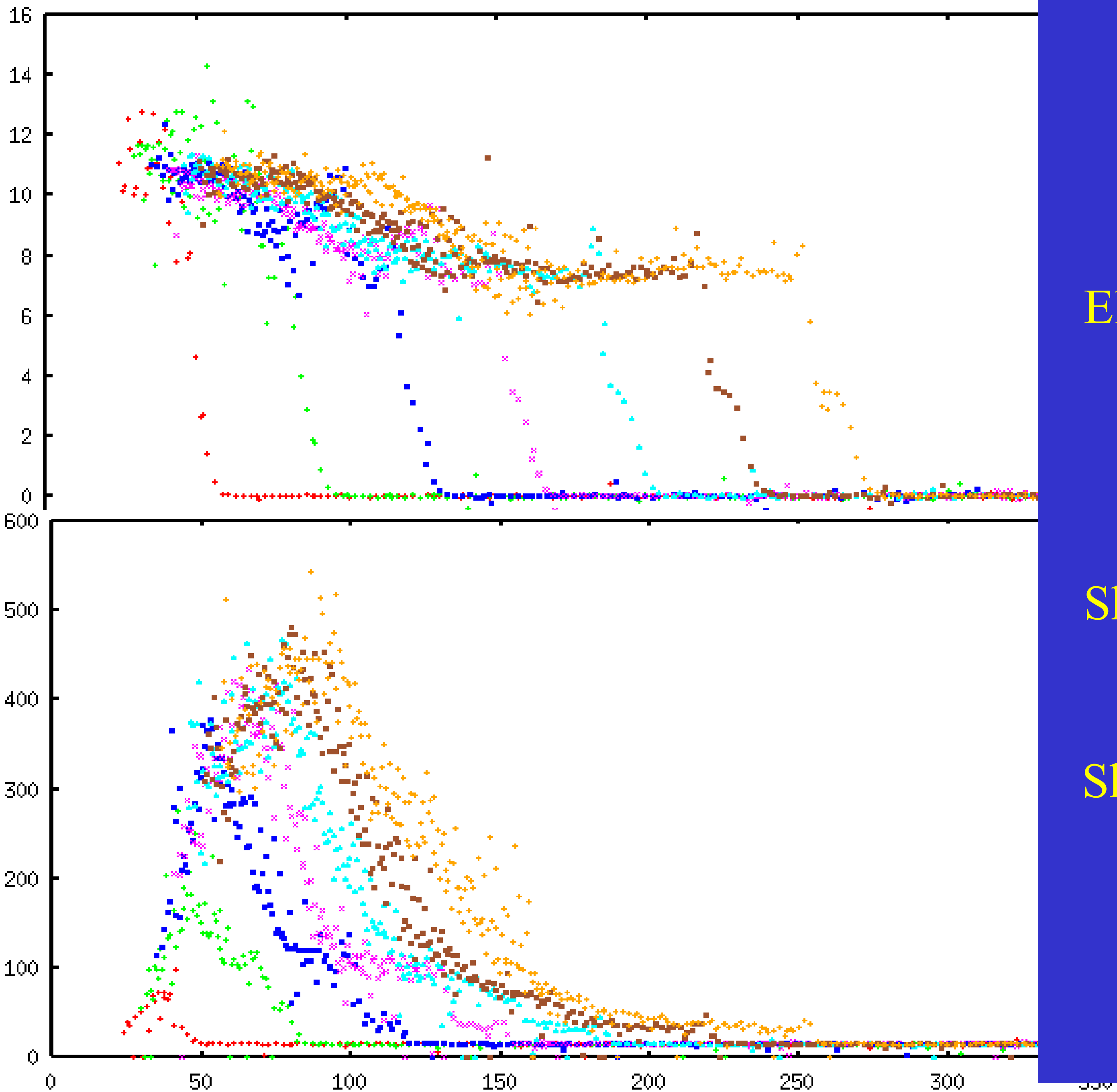
- **Lattice Constants**

	a (Å)	c (Å)	E (eV)	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
MEAM								
hcp	2.95	4.68	-5.019	183	94	72	191	50
omega	4.58	2.82	-5.015	197	87	56	234	35
bcc	3.27	—	-4.910	96	108	—	—	39
GGA								
hcp	2.95	4.67	-5.171	176	87	68	191	51
omega	4.59	2.84	-5.176	194	81	54	245	54
bcc	3.26	—	-5.063	95	110	—	—	41.7

- **Defect Energies**

Defect	MEAM (eV)	GGA (eV)
hcp		
Octahedral	2.242	2.58
Tetrahedral	unstable to dumbbell-0001	
Dumbbell-0001	2.346	2.87
Vacancy	1.557	2.03
Divacancy-AB	2.828	3.92
omega		
Octahedral	2.482	3.76
Tetrahedral	3.084	3.50
Vacancy-A	1.720	2.92
Vacancy-B	0.111	1.57





SHOCK (I)

Piston Velocity

1.1 km/s

Elastic Shock Wave Speed:

7.0 km/s

Transformation Shock Wave Speed:

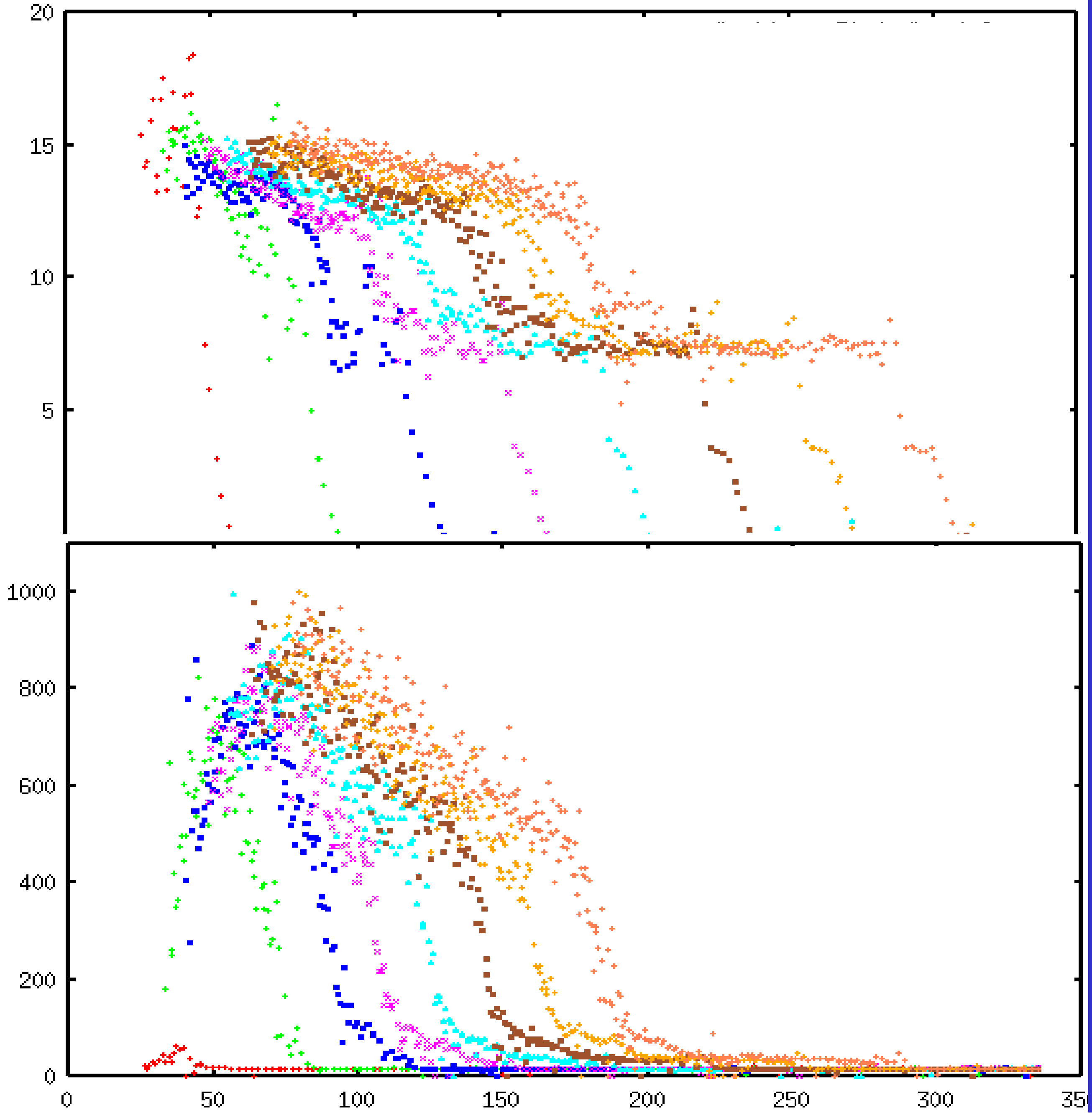
2.2 km/s

Shock Temperature:

450 K

Shock Pressure:

27 GPa



SHOCK (II)

PistonVelocity

1.5 km/s

Elastic Shock Wave Speed:

7.0 km/s

Transformation Shock Wave Speed:

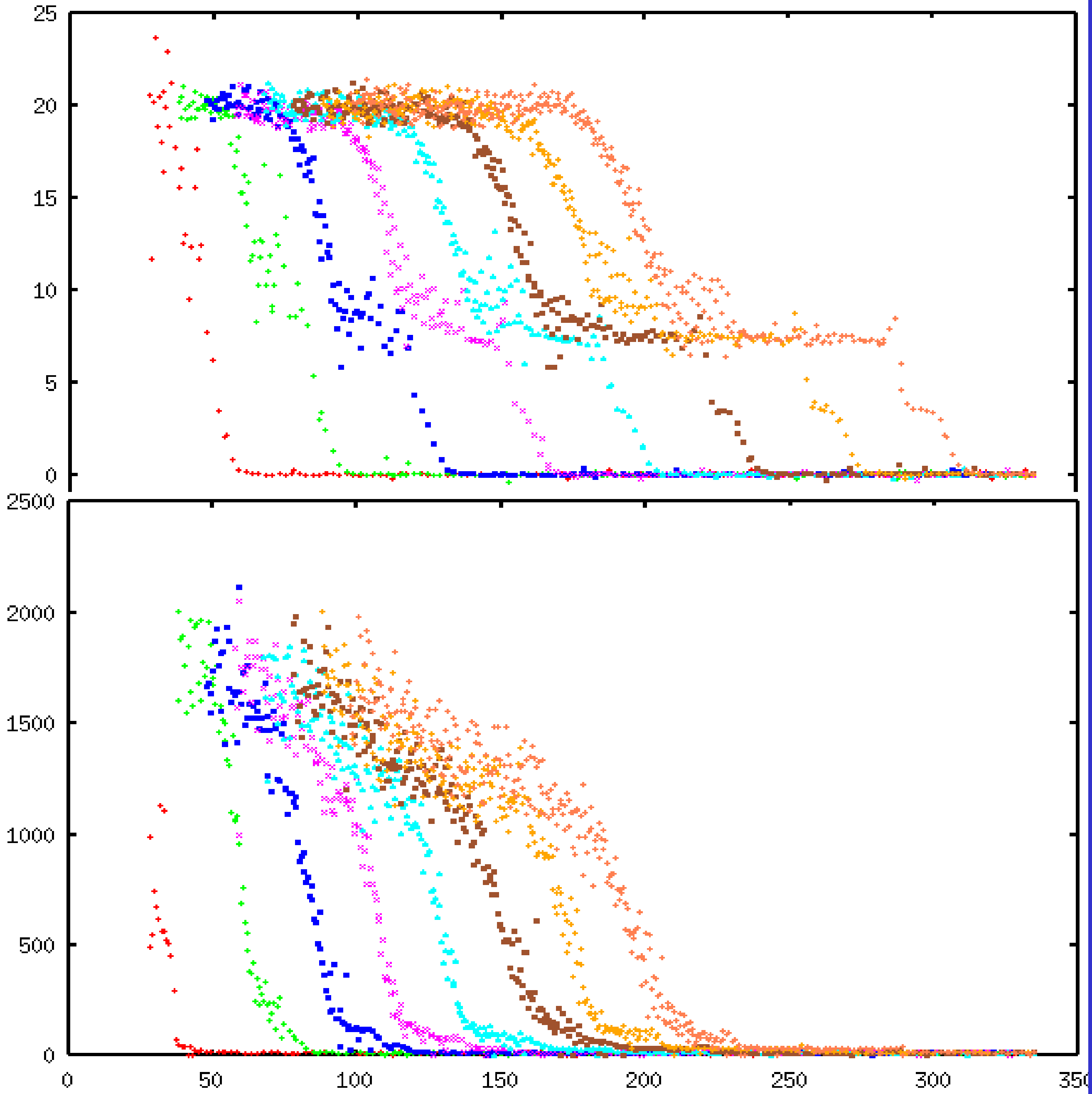
3.6 km/s

Shock Temperature:

900 K

Shock Pressure:

43 GPa



SHOCK (III)

Piston Velocity

2.0 km/s

Elastic Shock Wave Speed:

7.0 km/s

Transformation Shock Wave Speed:

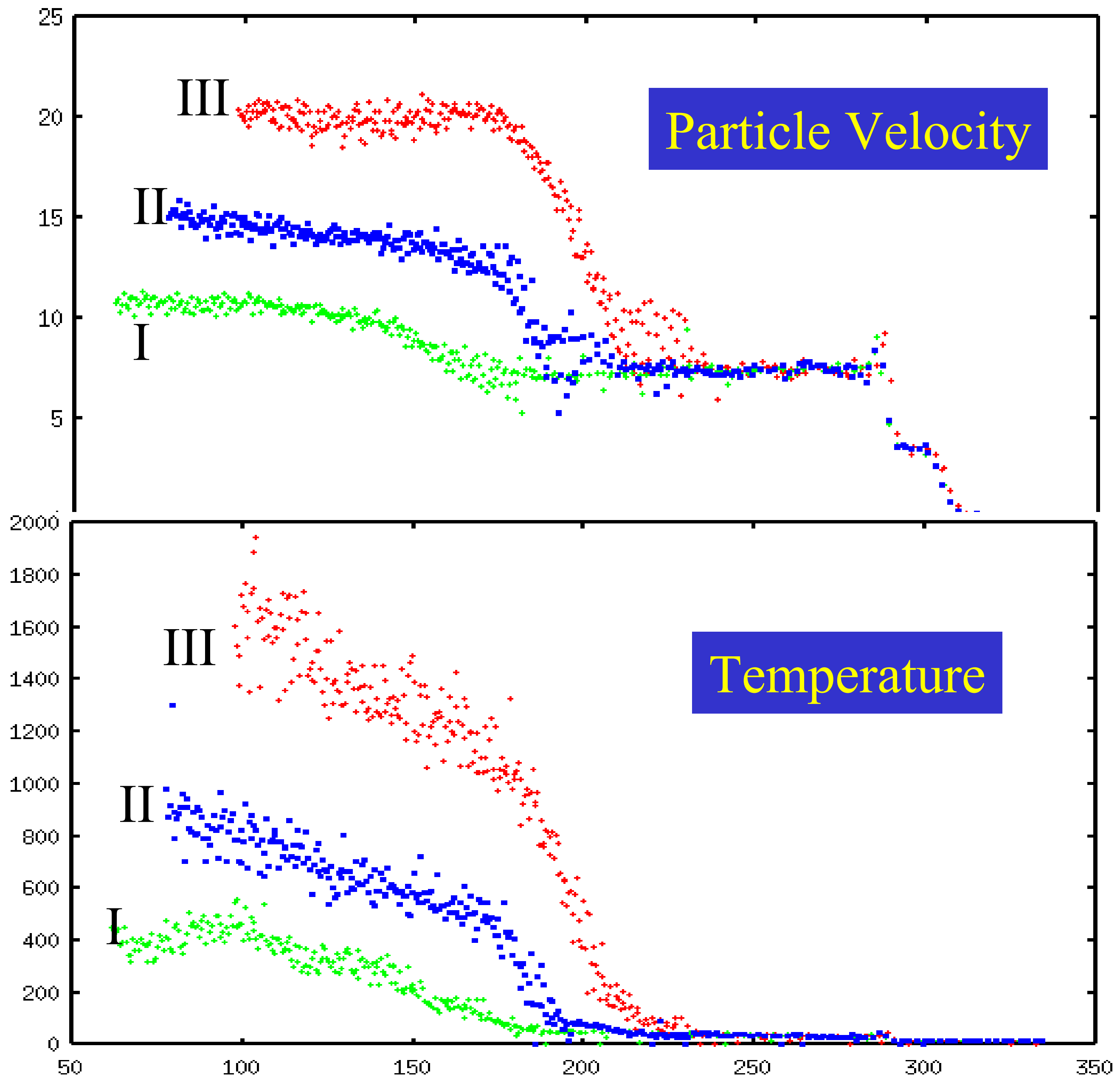
4.2 km/s

Shock Temperature:

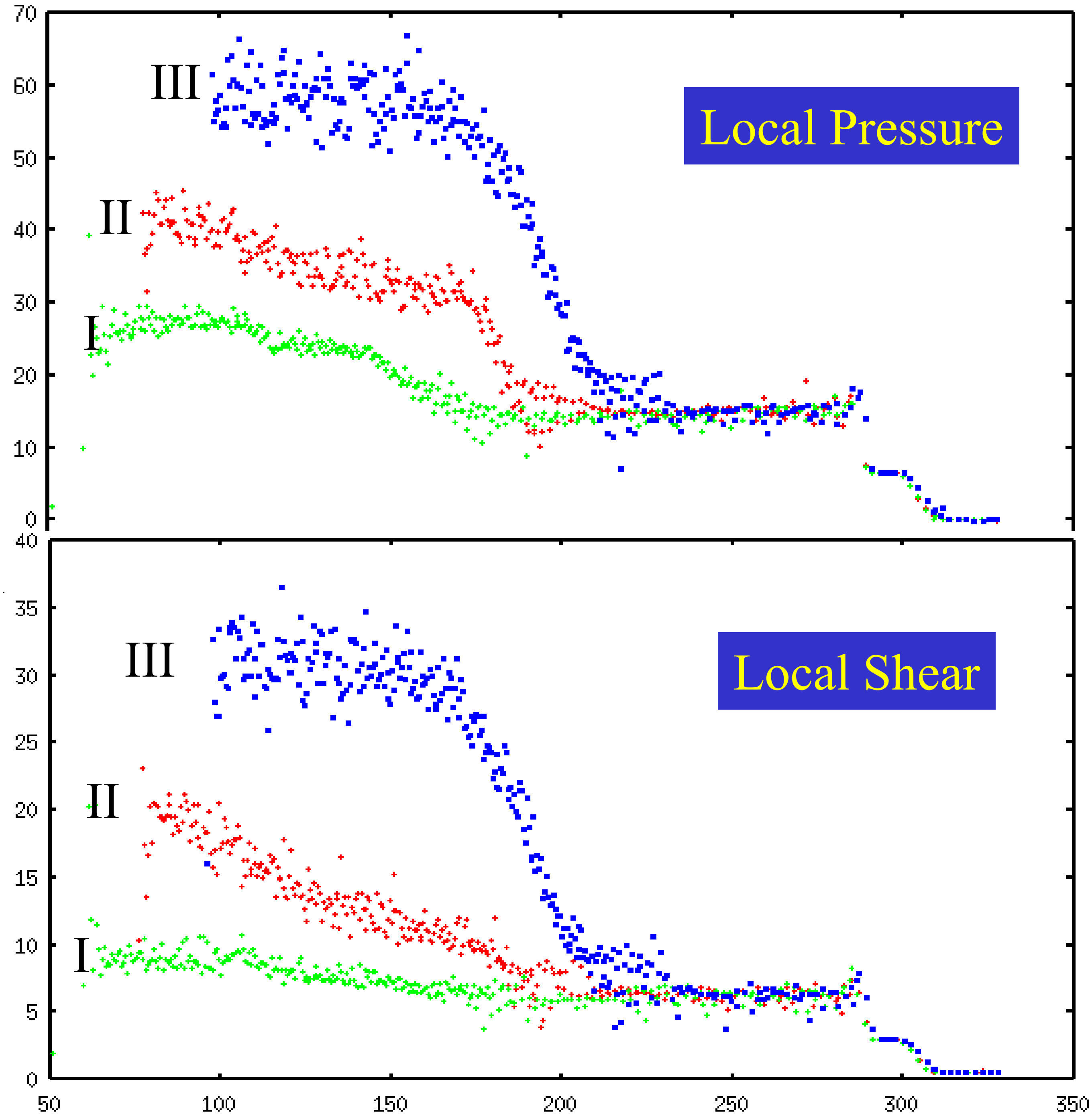
1800 K

Shock Pressure:

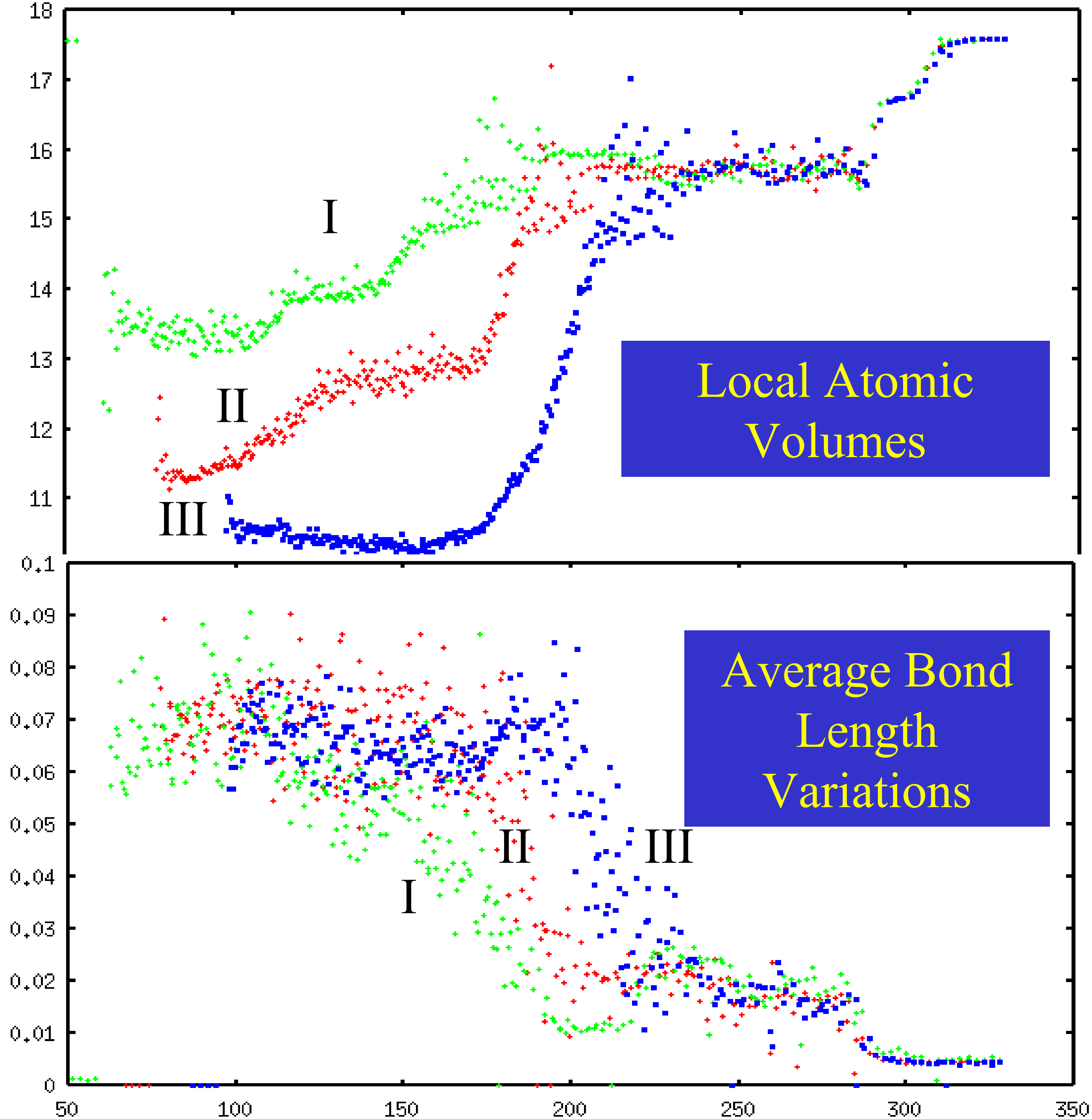
60 GPa



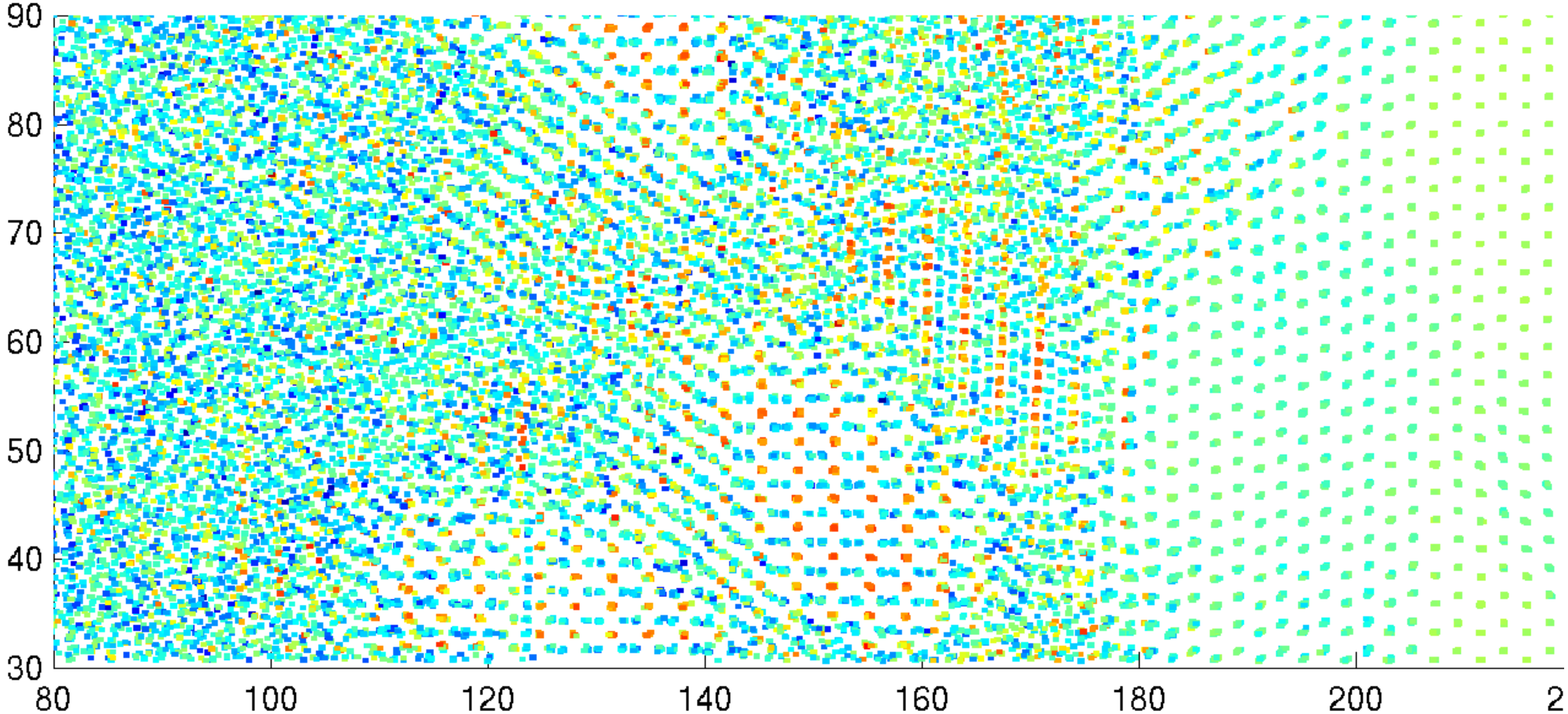
Particle Velocity
Temperature
III
II
I
25
20
15
10
5
2000
1800
1600
1400
1200
1000
800
600
400
200
0
50
100
150
200
250
300
350



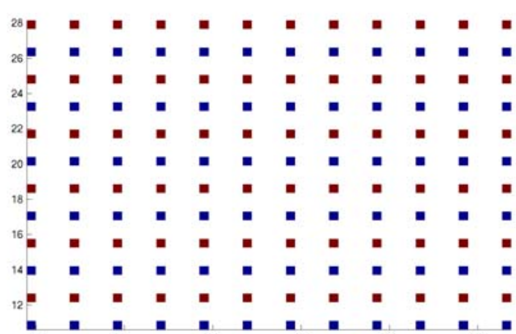
Local Pressure
III
II
I
Local Shear
III
II
I
70
60
50
40
30
20
10
0
40
35
30
25
20
15
10
5
0
50
100
150
200
250
300
350


Local Atomic Volumes
I
II
III
18
17
16
15
14
13
12
11
Average Bond Length Variations
I
II
III
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
50
100
150
200
250
300
350

The yz-view of the whole sample



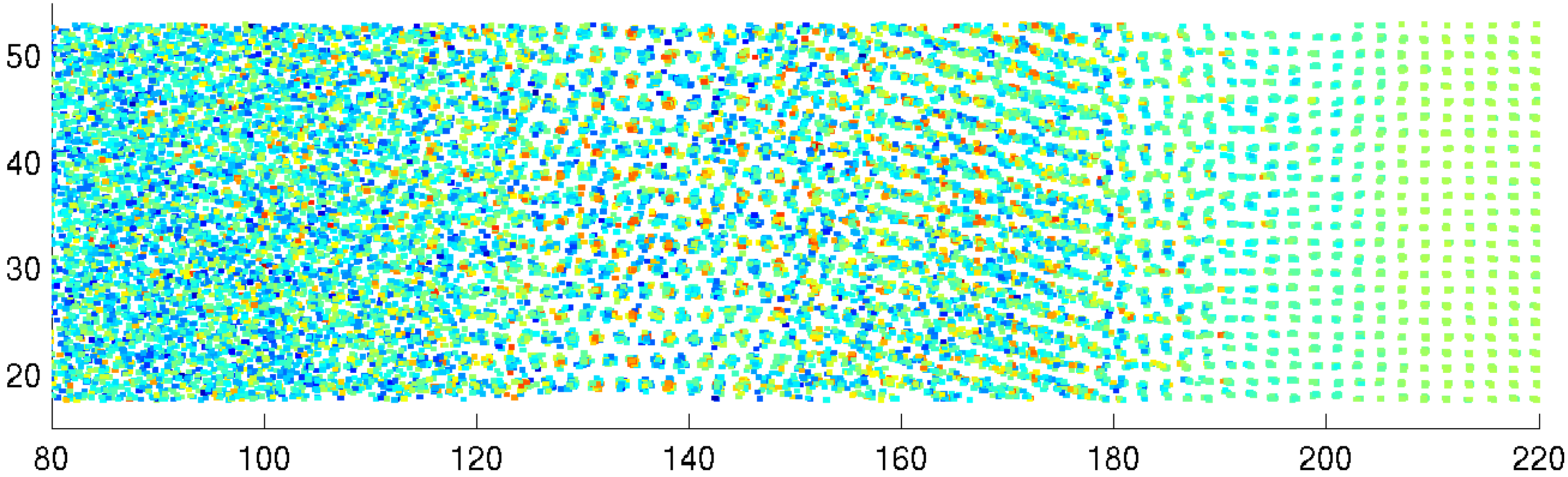
Omega phase



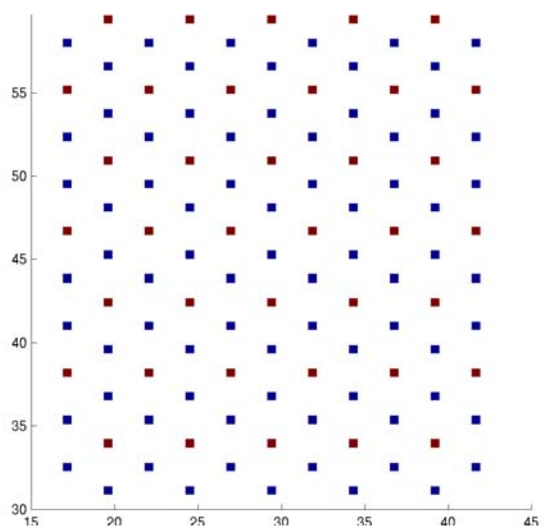
Coordination: 14

Coordination: 9

The xz-view of the whole sample



Omega phase



Coordination: 14

Coordination: 9